

17.0 Chemical Properties

Chemical properties are required by most of the modules of the 3MRA modeling system. This section describes how chemical properties were collected for the representative national data set included in the modeling system.

17.1 Parameters Collected

The chemical properties used by the 3MRA modeling system are listed in Table 17-1 along with the modules that use them.¹ Chemical properties are applied nationally and adjusted based on site-specific or regional pH and temperature conditions.

17.2 Data Sources and Methodology

The chemical property values used in the 3MRA modeling system were obtained through a combination of modeling, existing databases, and literature review. Table 17-2 summarizes how the various chemical properties were obtained. Certain metal partition coefficients, biodegradation rates, and hydrolysis rate constants were collected through literature surveys for measured values. Thermodynamic properties and partition coefficients for organic chemicals were calculated using the SPARC (System Performs Automated Reasoning in Chemistry) model and metal sorption isotherms were calculated using the MINTEQA2 geochemical speciation model. These models are described briefly below, along with their application for 3MRA modeling system.

SPARC. EPA developed the predictive modeling system SPARC to help meet the growing need for chemical-specific inputs for multimedia, multipathway, multireceptor risk assessment tools such as the 3MRA modeling system. SPARC (U.S. EPA, 2003) calculates a large number of physical and chemical parameters from chemical molecular structure and basic information about the environment (media, temperature, pressure, pH, etc.). For the 3MRA modeling system, SPARC is used to estimate solubility, vapor pressure, Henry's law constant, octanol/water partition coefficient, air diffusivity, water diffusivity, and ionization potential at a standard temperature and pH. These properties are contained in the 3MRA modeling system in text files. The Chemical Properties Processor (CPP; U.S. EPA, 1999d) reads those files to prepare the input files for the system modules. Prior to creating the input data sets, the CPP

¹ Chemical-specific bio-uptake, bioconcentration, and bioaccumulation factors used by the food web modules (Farm Food Chain, Terrestrial Food Web, and Aquatic Food Web Modules) are described in Chapter 10 of this volume.

Table 17-1. Chemical Properties by Module

| Chemical property | CPP ^a | Source Modules | | | | | Media Modules | | | Food Modules | |
|---|------------------|----------------|--------------|-----------|------------|-----|---------------|---------------|----------------|----------------------|------------------|
| | | Surface Imp. | Aerated Tank | Land-fill | Waste-pile | LAU | Water-shed | Surface Water | Vadose/Aquifer | TFW/FFC ^b | AFW ^c |
| <i>Thermodynamic Properties (organic chemicals)</i> | | | | | | | | | | | |
| Molecular weight | ● | | | | | | | ● | | | |
| Density | ● | | | | | | | ● | | | |
| Molecular volume | ● | | | | | | | ● | | | |
| Boiling point | ● | | | | | | | | | | |
| Vapor pressure | ○ | | | | | | | ● | | | |
| Solubility | ○ | ● | ● | ● | | | ● | ● | ● | | |
| Air diffusivity | ○ | ● | ● | ● | | | ● | ● | ● | | |
| Water diffusivity | ○ | ● | ● | ● | | | ● | ● | ● | | |
| Ionization coefficient | ● | | | | | | | | | | |
| <i>Partition Coefficients (organic chemicals)</i> | | | | | | | | | | | |
| Henry's law constant | ○ | ● | ● | ● | ● | ● | ● | ● | | ● | |
| Octanol-water partition coefficient | ○ | | | | | | | ● | | ● | ● |
| Soil-water partition coefficient | ○ | ● | ● | ● | ● | ● | ● | ● | ● | ● | |
| <i>Degradation Constants (organic chemicals)</i> | | | | | | | | | | | |
| Hydrolysis rates | ○ | ● | ● | ● | ● | ● | ● | ● | ● | | |
| Aerobic biodegradation rates | ● | ● | ● | ● | ● | ● | ● | ● | ● | | |
| Anaerobic biodegradation rates | ● | ● | ● | ● | ● | ● | ● | ● | ● | | |
| <i>Partition Coefficients (metals)</i> | | | | | | | | | | | |
| Partition coefficients (waste, soil, surface water, sediment) | ● | ● | ● | ● | ● | ● | ● | ● | | | |
| Sorption isotherms | | | | | | | | | ● | | |

^a Chemical Properties Processor^b TFW = terrestrial food web

FFC = farm food chain

^c AFW = aquatic food web

○ calculated and/or adjusted for media pH and temperature conditions by the CPP

● used directly without adjustment

adjusts the SPARC-calculated properties to the temperature and pH conditions for the site and media being modeled. The CPP also calculates soil-water partition coefficients from octanol-water partition coefficients. U.S. EPA (1999c) describes the algorithms used within the CPP for these adjustments and calculations.

Table 17-2. Methodology and Data Sources for 3MRA Chemical Properties

| Property | Methodology | References |
|--|--|-------------------------------------|
| Organic Chemicals | | |
| Thermodynamic properties and partition coefficients ^a | SPARC-calculated values, adjusted by CPP for temperature and pH | U.S. EPA (2003) U.S. EPA (1999c) |
| Hydrolysis rates | Measured or estimated rate constants adjusted by CPP for temperature and pH | U.S. EPA (1996) U.S. EPA (1999c) |
| Aerobic biodegradation rates | Measured values from literature, grouped by pH and temperature regimes | Aronson et al. (1999) |
| Anaerobic biodegradation rates | Measured values from literature, grouped by pH, temperature, and redox regimes | U.S. EPA (1999a) |
| Soil/water partition coefficients | Calculated from Kow by CPP | U.S. EPA (1999c) |
| Metals | | |
| Partition coefficients (waste, soil, surface water, sediment) | Measured or estimated values, presented as national distributions | U.S. EPA (1999e) |
| Sorption isotherms | MINTEQA2 model | U.S. EPA (1998, 1999b) |

^a molecular weight, density, volume, vapor pressure, boiling point, air and water diffusion coefficients, solubility, Henry's law constant, octanol/water partition coefficient (Kow), ionization coefficient

MINTEQA2. The MINTEQA2 model was used to develop metal sorption isotherms that are contained within the Vadose Zone and Aquifer Modules and used to provide the pH and concentration-adjusted soil-water partition coefficients needed to estimate sorption of metal contaminants in the subsurface. MINTEQA2 is a equilibrium speciation model that calculates the equilibrium composition of dilute aqueous solutions in the laboratory or in natural aqueous systems. The model can calculate the equilibrium mass distribution among dissolved species, adsorbed species, and multiple solid phases under a variety of conditions, including a gas phase with constant partial pressure. For more information on MINTEQA2, see U.S. EPA (1998) and U.S. EPA (1999b).

Other chemical properties were obtained from literature sources or estimated using empirical methods and expert judgment. Anaerobic and aerobic biodegradation rates and degradation products were collected using preestablished criteria for the evaluation of field and laboratory studies (U.S. EPA, 1999a; Aronson et al., 1999). The collected biodegradation rates are grouped by pH and temperature regimes and the CPP selects the appropriate value depending on media pH and temperature conditions at a site, or within a waste management unit. Anaerobic degradation rates are also grouped by redox regime (reducing, sulfate reducing, and methanogenic), which can be randomly selected during Monte Carlo runs.

Hydrolysis rates were compiled by EPA scientists along with probable pathways and degradation products for the hydrolysis reactions in question (U.S. EPA, 1996). EPA used literature sources where available, and supplemented these published data with laboratory experiments and expertise in structure activity relationships as needed. The overall hydrolysis rate constants used by the 3MRA modeling system are calculated by the CPP as a summation of the rate constants for acid, neutral, and base hydrolysis, using site-specific pH and temperature conditions in the media being modeled (U.S. EPA, 1999c).

The metal sorption coefficients for surface soils, surface water, sediments, and wastes were collected from literature where available, or estimated using a combination of empirical relationships with available literature values, geochemical modeling using MINTEQA2, and expert judgment. The methodology employed to collect or estimate these metal Kd values is described in detail in U.S. EPA (1999e). To represent the nationwide variability in sorption coefficients, the metal Kd values for each media are contained within the 3MRA modeling system as distributions that are randomly sampled by the CPP during model execution.

17.3 Quality Assurance/Quality Control

Quality assurance/quality control (QA/QC) protocols were developed and followed for each chemical property data collection effort. These QA/QC protocols are described in the documents referenced in Section 17.2.

17.4 Results

Appendix 17A provides the chemical property values included in the 3MRA modeling system for the 46 chemicals in the representative national data set. These values are contained in a set of text (.csv) files. During model execution, these files are read by the CPP to provide the appropriate chemical property data to each module. Table 17-3 lists the text files and the chemical properties that they contain.

Table 17-3. Chemical Property Files Contained within 3MRA Modeling System

| File Name | Contents |
|-------------|---|
| AerBio.csv | Aerobic biodegradation rate constants (minimum, maximum, central tendency, standard deviation, and distribution type); reaction products |
| AnaBio.csv | Anaerobic biodegradation rate constants (minimum, maximum, central tendency, standard deviation, and distribution type); reaction products |
| AnaRed.csv | Anaerobic biodegradation rate constants, reducing redox regime (minimum, maximum, central tendency, standard deviation, and distribution type); reaction products |
| CAT.csv | Catalyzed acid, neutral, and base hydrolysis rates; reaction products |
| MethBio.csv | Anaerobic biodegradation rate constants, methanogenic redox regime (minimum, maximum, central tendency, standard deviation, and distribution type); reaction products |
| MICP.csv | Metal sorption coefficients (minimum, maximum, central tendency, standard deviation, and distribution type) |
| OCP.csv | Organic chemical thermodynamic properties and partition coefficients |
| SO4Bio.csv | Anaerobic biodegradation rate constants, sulfate-reducing redox regime (minimum, maximum, central tendency, standard deviation, and distribution type); reaction products |

17.5 Issues and Uncertainties

Issues and uncertainties associated with the various chemical properties in the representative national data set can be found in the documentation listed for each property in Section 17.2.

17.6 References

- Aronson, D., M. Citra, K. Schuler, H. Printup, and P.H. Howard. 1999. *Aerobic Biodegradation of Organic Chemicals in Environmental Media: A Summary of Field and Laboratory Studies*. SRC TR 99-002. Syracuse Research Corporation. Syracuse, NY.
- U.S. EPA (Environmental Protection Agency). 1996. *Environmental Fate Constants for Organic Chemicals under Consideration for EPA's Hazardous Waste Identification Rule*. Office of Research and Development. Athens, GA.
- U.S. EPA (Environmental Protection Agency). 1998. *MINTEQA2/PRODEFA2, A Geochemical Assessment Model for Environmental Systems: User Manual Supplement for Version 4.0*. Prepared for the U.S. Environmental Protection Agency by HydroGeoLogic, Inc., Contract No. 68-C6-0020.
- U.S. EPA (Environmental Protection Agency). 1999a. *Anaerobic Biodegradation of Organic Chemicals in Groundwater: Summary of Field and Laboratory Studies*. Office of Solid Waste. Washington, DC.
- U.S. EPA (Environmental Protection Agency). 1999b. *Changes in the MINTEQA2 Modeling Procedure for Estimating Metal Partition Coefficients in Groundwater*, prepared by HydroGeoLogic, Inc. for the U.S. Environmental Protection Agency, Washington, DC.
- U.S. EPA (Environmental Protection Agency). 1999c. *Chemical Database for HWIR99*. Office of Solid Waste. Athens, GA.
- U.S. EPA (Environmental Protection Agency). 1999d. *Documentation for the FRAMES-HWIR Technology Software System, Volume 13: Chemical Properties Processor*. Office of Research and Development. Athens, GA.
- U.S. EPA (Environmental Protection Agency). 1999e. *Surface Water, Soil, and Waste Partition Coefficients for Metals*. Office of Solid Waste. Washington, DC.
- U.S. EPA (Environmental Protection Agency). 2003. *Prediction of Chemical Reactivity Parameters and Physical Properties of Organic Compounds from Molecular Structure Using SPARC*. Internal Report. Ecosystems Research Division, National Exposure Research Laboratory, Athens, GA. March.

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Appendix 17A

Chemical Properties Values in the 3MRA Modeling System Representative National Data Set

| | | |
|---------------|--|-------|
| Table 17A-1. | Organic Chemical Properties | 17-9 |
| Table 17A-2a. | Chemical Properties for Metals | 17-11 |
| Table 17A-2b. | Metal Partition Coefficients | 17-12 |
| Table 17A-3. | Aerobic Biodegradation Rates | 17-16 |
| Table 17A-4. | Anaerobic Biodegradation Rates | 17-17 |
| Table 17A-5. | Anaerobic Biodegradation Rates, Reducing Conditions | 17-18 |
| Table 17A-6a. | Anaerobic Biodegradation Rates: Methanogenic Conditions | 17-19 |
| Table 17A-6b. | Anaerobic Biodegradation Rates: Methanogenic Conditions | 17-20 |
| Table 17A-7. | Anaerobic Biodegradation Rates - Sulfate Reducing Conditions | 17-22 |
| Table 17A-8. | Catalyzed Hydrolysis Rates | 17-25 |

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Table 17A-1. Organic Chemical Properties

| Chemical | MW | AirDif | Volume | VP | Ka1 | Sol | HLC | Kow |
|--|--------|--------------------|----------|-----------|-------|-----------|-------------------------|-----------|
| | g/mole | cm ² /s | mL | torr | mg/L | mg/L | atm m ³ /mol | mL/mL |
| Acetonitrile | 41.05 | 2.37E-06 | 2.57E+01 | 8.96E+00 | NA | 4.80E+00 | 2.89E+00 | 1.61E+00 |
| Acrylonitrile | 53.06 | 1.59E-06 | 3.94E+01 | 1.14E+01 | NA | 6.12E+00 | 4.08E+00 | 1.57E+00 |
| Aniline | 93.13 | 1.30E-06 | 7.28E+01 | 8.54E+00 | 0.234 | 7.51E+00 | 1.16E-01 | -9.47E-01 |
| Benzene | 78.11 | 1.71E-06 | 5.72E+01 | 8.17E+00 | NA | 5.78E+00 | 1.40E+00 | 3.80E-01 |
| Benzo(a)pyrene | 252.31 | 5.14E-07 | 1.99E+02 | -4.60E+00 | NA | 3.33E+00 | -8.30E+00 | 4.67E+00 |
| Bis-(2-ethylhexyl) phthalate | 390.56 | 4.07E-07 | 3.24E+02 | -7.20E+00 | NA | 3.64E+00 | -1.04E+01 | 3.55E+00 |
| Carbondisulfide | 76.14 | 2.19E-06 | 4.26E+01 | 7.51E+00 | NA | 1.63E+00 | 1.58E+00 | 4.41E-01 |
| Chlorobenzene | 112.56 | 1.34E-06 | 7.22E+01 | 7.21E+00 | NA | 5.52E+00 | 8.59E-01 | 6.06E-01 |
| Chloroform | 119.38 | 1.76E-06 | 4.87E+01 | 7.78E+00 | NA | 5.27E+00 | 1.71E+00 | 1.62E-01 |
| Dibenz(a,h)anthracene | 278.35 | 4.75E-07 | 2.13E+02 | -2.07E+01 | NA | -6.00E-01 | -1.94E+01 | 7.78E+00 |
| 2,4-D [2,4-Dichlorophenoxyacetic acid] | 221.04 | 7.96E-07 | 1.25E+02 | 6.90E+00 | 3.74 | 7.08E+00 | -7.04E-01 | -5.35E-02 |
| Ethylenedibromide | 187.86 | 1.36E-06 | 6.18E+01 | 8.12E+00 | NA | 5.86E+00 | 1.66E+00 | -1.28E-01 |
| Hexachloro-1,3-butadiene | 260.76 | 8.30E-07 | 1.17E+02 | 7.66E+00 | NA | 5.02E+00 | 2.17E+00 | 1.02E-01 |
| Methoxychlor | 345.65 | 5.23E-07 | 2.16E+02 | -7.25E-01 | NA | 4.50E+00 | -5.53E+00 | 4.27E+00 |
| Methylethylketone | 72.11 | 1.70E-06 | 5.41E+01 | 7.81E+00 | NA | 3.28E+00 | 3.51E+00 | 1.54E+00 |
| Methylmethacrylate | 100.12 | 1.40E-06 | 7.22E+01 | 7.95E+00 | NA | 4.05E+00 | 3.02E+00 | 1.05E+00 |
| Methylenechloride | 84.93 | 2.15E-06 | 3.70E+01 | 7.57E+00 | NA | 4.31E+00 | 1.31E+00 | 1.42E-01 |
| Nitrobenzene | 123.11 | 1.15E-06 | 7.78E+01 | 8.21E+00 | NA | 5.89E+00 | 1.53E+00 | 1.47E+00 |
| Pentachlorophenol | 266.34 | 8.25E-07 | 1.24E+02 | 7.32E+00 | 4.47 | 3.70E+00 | 3.15E+00 | 7.29E-01 |
| Phenol | 94.11 | 1.33E-06 | 7.04E+01 | 1.03E+01 | 4.47 | 9.60E+00 | -1.45E-01 | -2.00E+00 |

(continued)

Table 17A-1. (continued)

| Chemical | MW | AirDif | Volume | VP | Ka1 | Sol | HLC | Kow |
|--|-----------|--------------------|---------------|-----------|------------|------------|-------------------------|------------|
| | g/mole | cm ² /s | mL | torr | mg/L | mg/L | atm m ³ /mol | mL/mL |
| Pyridine | 79.1 | 1.62E-06 | 5.45E+01 | 8.22E+00 | 2.58 | 4.23E+00 | 3.01E+00 | 8.22E-01 |
| 2,3,7,8-Tetrachlorodibenzo-p-dioxin [2,3,7,8-TCDD] | 321.97 | 6.10E-07 | 1.75E+02 | -2.68E+00 | NA | 1.64E+00 | -4.90E+00 | 5.01E+00 |
| Tetrachloroethylene | 165.83 | 1.37E-06 | 7.31E+01 | 7.77E+00 | NA | 4.67E+00 | 2.44E+00 | 6.63E-01 |
| Thiram | 240.44 | 5.67E-07 | 1.70E+02 | 8.08E+00 | NA | 4.63E+00 | 2.94E+00 | -1.09E-01 |
| Toluene | 92.14 | 1.42E-06 | 7.19E+01 | 7.86E+00 | NA | 5.60E+00 | 1.34E+00 | 3.89E-01 |
| 1,1,1-Trichloroethane | 133.4 | 1.56E-06 | 6.95E+01 | 7.56E+00 | NA | 5.16E+00 | 1.65E+00 | 2.80E-01 |
| Trichloroethylene | 131.39 | 1.60E-06 | 6.11E+01 | 7.68E+00 | NA | 4.65E+00 | 2.27E+00 | 6.72E-01 |
| Vinylchloride | 62.5 | 2.57E-06 | 3.62E+01 | 7.17E+00 | NA | 4.87E-01 | 1.55E+00 | 5.55E-01 |

Properties generated by SPARC chemical properties estimator

MW = molecular weight; AirDif = air diffusivity; Volume = molar volume; VP = vapor pressure; Ka1 = ionization coefficient

Sol = solubility; HLC = Henry's Law constant; Kow = octanol/water partition coefficient; Koc = soil / water partition coefficient

NA = not available

Table 17A-2a. Chemical Properties for Metals (MICP.csv)

| Chemical | MW | Wdiff (mean) | Wdiff (min) | Wdiff (max) | Wdiff (dist) | Sol |
|-------------------|---------|--------------------|--------------------|--------------------|-----------------|----------|
| | g/mole | cm ² /s | cm ² /s | cm ² /s | - | mg/L |
| Antimony | 121.75 | - | 1.00E-04 | 1.00E-02 | Uniform | 1.00E+05 |
| Arsenic | 74.92 | - | 1.00E-04 | 1.00E-02 | Uniform | 1.00E+05 |
| Barium | 137.33 | - | 1.00E-04 | 1.00E-02 | Uniform | 1.00E+05 |
| Beryllium | 9.01218 | - | 1.00E-04 | 1.00E-02 | Uniform | 1.00E+05 |
| Cadmium | 112.4 | - | 1.00E-04 | 1.00E-02 | Uniform | 1.00E+05 |
| Chromium III | 52 | - | 1.00E-04 | 1.00E-02 | Uniform | 1.00E+05 |
| Chromium VI | 52 | - | 1.00E-04 | 1.00E-02 | Uniform | 1.00E+05 |
| Lead | 207.2 | - | 1.00E-04 | 1.00E-02 | Uniform | 1.00E+05 |
| Divalent mercury | 200 | 1.00E-04 | | | Constant | 1.00E+05 |
| Elemental mercury | 200 | 1.00E-04 | | | Constant | 2.50E-02 |
| Methyl mercury | 215 | 1.00E-04 | | | Constant | 1.00E+05 |
| Nickel (+2) | 58.7 | - | 1.00E-04 | 1.00E-02 | Uniform | 1.00E+05 |
| Selenium (+6) | 78.96 | - | 1.00E-04 | 1.00E-02 | Uniform | 1.00E+05 |
| Silver | 107.87 | - | 1.00E-04 | 1.00E-02 | Uniform | 1.00E+05 |
| Thallium | 204.37 | - | 1.00E-04 | 1.00E-02 | Uniform | 1.00E+05 |
| Vanadium | 50.9415 | - | 1.00E-04 | 1.00E-02 | Uniform | 1.00E+05 |
| Zinc | 65.38 | - | 1.00E-04 | 1.00E-02 | Uniform | 1.00E+05 |

MW = molecular weight; Wdiff = water diffusivity

Sol = solubility limit for sediment, soil, and wastes in LAUs, waste piles, surface impoundments, and aerated tanks

Table 17A-2b. Metal Partition Coefficients (Kd values; MICP.csv)

| Chemical | Statistic | Environmental Media Kd Values (L/kg) | | | | Waste Kd Values (L/kg) | | | | |
|-----------|-----------|--------------------------------------|------------|------------|---------------|------------------------|------------|------------|---------------------|--------------|
| | | Organic carbon | Soil | Sediment | Surface Water | LAU | Waste Pile | Landfill | Surface Impoundment | Aerated Tank |
| Antimony | min | 0 | 1.258925 | 3.981072 | 7943.282 | 1.00714 | 1.00714 | 1.00714 | 7943.282347 | 7943.282 |
| | mean | 5.01E+02 | 199.5262 | 3981.072 | 63095.73 | 159.621 | 159.621 | 159.621 | 63095.73445 | 63095.73 |
| | max | 2.00E+04 | 501.1872 | 63095.73 | 79432.82 | 400.9498 | 400.9498 | 400.9498 | 79432.82347 | 79432.82 |
| | std. dev. | | 12.58925 | 63.09573 | 3.162278 | 10.0714 | 10.0714 | 10.0714 | 3.16227766 | 3.162278 |
| | distrib. | constant | triangular | triangular | triangular | triangular | triangular | triangular | triangular | triangular |
| Arsenic | min | | 1.995262 | 39.81072 | 100 | 1.59621 | 1.59621 | 1.59621 | 100 | 100 |
| | mean | 0 | 1584.893 | 251.1886 | 7943.282 | 1267.915 | 1267.915 | 1267.915 | 7943.282347 | 7943.282 |
| | max | | 19952.62 | 19952.62 | 1000000 | 15962.1 | 15962.1 | 15962.1 | 1000000 | 1000000 |
| | std. dev. | | 5.011872 | 5.011872 | 3.162278 | 4.009498 | 4.009498 | 4.009498 | 3.16227766 | 3.162278 |
| | distrib. | constant | triangular | triangular | triangular | triangular | triangular | triangular | triangular | triangular |
| Barium | min | | 5.011872 | 7.943282 | 794.3282 | 4.009498 | 4.009498 | 4.009498 | 794.3282347 | 794.3282 |
| | mean | 0 | 100 | 316.2278 | 10000 | 80 | 80 | 80 | 10000 | 10000 |
| | max | | 2511.886 | 1584.893 | 31622.78 | 2009.509 | 2009.509 | 2009.509 | 31622.7766 | 31622.78 |
| | std. dev. | | 5.011872 | 6.309573 | 2.511886 | 4.009498 | 4.009498 | 4.009498 | 2.511886432 | 2.511886 |
| | distrib. | constant | triangular | triangular | triangular | triangular | triangular | triangular | triangular | triangular |
| Beryllium | min | 1.00E+03 | 50.11872 | 6.309573 | 630.9573 | 40.09498 | 40.09498 | 40.09498 | 630.9573445 | 630.9573 |
| | mean | 3.16E+04 | 158.4893 | 630.9573 | 15848.93 | 126.7915 | 126.7915 | 126.7915 | 15848.93192 | 15848.93 |
| | max | 2.00E+05 | 12589.25 | 3162278 | 6309573 | 10071.4 | 10071.4 | 10071.4 | 6309573.445 | 6309573 |
| | std. dev. | | 10 | 79.43282 | 5.011872 | 8 | 8 | 8 | 5.011872336 | 5.011872 |
| | distrib. | constant | triangular | triangular | triangular | triangular | triangular | triangular | triangular | triangular |

(continued)

Table 17A-2b. (continued)

| Chemical | Statistic | Environmental Media Kd Values (L/kg) | | | | Waste Kd Values (L/kg) | | | | |
|------------------|-----------|--------------------------------------|------------|------------|---------------|------------------------|------------|------------|---------------------|--------------|
| | | Organic carbon | Soil | Sediment | Surface Water | LAU | Waste Pile | Landfill | Surface Impoundment | Aerated Tank |
| Cadmium | min | 2.51E+03 | 1.258925 | 3.162278 | 630.9573 | 1.00714 | 1.00714 | 1.00714 | 630.9573445 | 630.9573 |
| | mean | 1.58E+05 | 501.1872 | 1995.262 | 79432.82 | 400.9498 | 400.9498 | 400.9498 | 79432.82347 | 79432.82 |
| | max | 3.16E+05 | 100000 | 19952623 | 1995262 | 80000 | 80000 | 80000 | 1995262.315 | 1995262 |
| | std. dev. | | 6.309573 | 63.09573 | 3.981072 | 5.047659 | 5.047659 | 5.047659 | 3.981071706 | 3.981072 |
| | distrib. | constant | triangular | triangular | triangular | triangular | triangular | triangular | triangular | triangular |
| Chromium III | min | | 10 | 79.43282 | 7943.282 | 8 | 8 | 8 | 7943.282347 | 7943.282 |
| | mean | 0 | 6309.573 | 79432.82 | 125892.5 | 5047.659 | 5047.659 | 5047.659 | 125892.5412 | 125892.5 |
| | max | | 50118.72 | 794328.2 | 1000000 | 40094.98 | 40094.98 | 40094.98 | 1000000 | 1000000 |
| | std. dev. | | 2.511886 | 31.62278 | 2.511886 | 2.009509 | 2.009509 | 2.009509 | 2.511886432 | 2.511886 |
| | distrib. | constant | triangular | triangular | triangular | triangular | triangular | triangular | triangular | triangular |
| Chromium VI | min | | 0.199526 | 1 | 3981.072 | 0.159621 | 0.159621 | 0.159621 | 3981.071706 | 3981.072 |
| | mean | 0 | 6.309573 | 50.11872 | 15848.93 | 5.047659 | 5.047659 | 5.047659 | 15848.93192 | 15848.93 |
| | max | | 1995.262 | 25118.86 | 125892.5 | 1596.21 | 1596.21 | 1596.21 | 125892.5412 | 125892.5 |
| | std. dev. | | 6.309573 | 25.11886 | 3.162278 | 5.047659 | 5.047659 | 5.047659 | 3.16227766 | 3.162278 |
| | distrib. | constant | triangular | triangular | triangular | triangular | triangular | triangular | triangular | triangular |
| Divalent mercury | min | 1.00E+04 | 158.4893 | 6309.573 | 15848.93 | 126.7915 | 126.7915 | 126.7915 | 15848.93192 | 15848.93 |
| | mean | 5.00E+04 | 3981.072 | 79432.82 | 199526.2 | 3184.857 | 3184.857 | 3184.857 | 199526.2315 | 199526.2 |
| | max | 1.00E+05 | 630957.3 | 1000000 | 7943282 | 504765.9 | 504765.9 | 504765.9 | 7943282.347 | 7943282 |
| | std. dev. | | 5.011872 | 3.981072 | 2.511886 | 4.009498 | 4.009498 | 4.009498 | 2.511886432 | 2.511886 |
| | distrib. | triangular | triangular | triangular | triangular | triangular | triangular | triangular | triangular | triangular |

(continued)

Table 17A-2b. (continued)

| Chemical | Statistic | Environmental Media Kd Values (L/kg) | | | | Waste Kd Values (L/kg) | | | |
|-------------------|-----------|--------------------------------------|------------|------------|---------------|------------------------|------------|------------|---------------------|
| | | Organic carbon | Soil | Sediment | Surface Water | LAU | Waste Pile | Landfill | Surface Impoundment |
| Elemental mercury | min | 1.00E-03 | 158.4893 | 6309.573 | 15848.93 | 126.7915 | 126.7915 | 126.7915 | 15848.93192 |
| | mean | 1.00E-03 | 3981.072 | 79432.82 | 199526.2 | 3184.857 | 3184.857 | 3184.857 | 199526.2315 |
| | max | 1.00E+00 | 630957.3 | 1000000 | 7943282 | 504765.9 | 504765.9 | 504765.9 | 7943282.347 |
| | std. dev. | | 3.162278 | 3.981072 | 2.511886 | 2.529822 | 2.529822 | 2.529822 | 2.511886432 |
| | distrib. | triangular | triangular | triangular | triangular | triangular | triangular | triangular | triangular |
| Lead | min | 6.31E+03 | 5.011872 | 100 | 2511.886 | 4.009498 | 4.009498 | 4.009498 | 2511.886432 |
| | mean | 1.26E+05 | 5011.872 | 39810.72 | 501187.2 | 4009.498 | 4009.498 | 4009.498 | 501187.2336 |
| | max | 3.98E+05 | 100000 | 10000000 | 3162278 | 80000 | 80000 | 80000 | 3162277.66 |
| | std. dev. | | 15.84893 | 79.43282 | 2.511886 | 12.67915 | 12.67915 | 12.67915 | 2.511886432 |
| | distrib. | constant | triangular | triangular | triangular | triangular | triangular | triangular | triangular |
| Methyl mercury | min | 5.00E+04 | 19.95262 | 630.9573 | 15848.93 | 15.9621 | 15.9621 | 15.9621 | 15848.93192 |
| | mean | 1.00E+05 | 501.1872 | 7943.282 | 79432.82 | 400.9498 | 400.9498 | 400.9498 | 79432.82347 |
| | max | 5.00E+05 | 63095.73 | 100000 | 1584893 | 50476.59 | 50476.59 | 50476.59 | 1584893.192 |
| | std. dev. | | 3.981072 | 3.162278 | 5.011872 | 3.184857 | 3.184857 | 3.184857 | 5.011872336 |
| | distrib. | Triangular | triangular | triangular | triangular | triangular | triangular | triangular | triangular |
| Nickel (+2) | min | 5.01E+04 | 10 | 1.995262 | 3162.278 | 8 | 8 | 8 | 3162.27766 |
| | mean | 1.26E+05 | 794.3282 | 7943.282 | 25118.86 | 635.4626 | 635.4626 | 635.4626 | 25118.86432 |
| | max | 2.51E+05 | 6309.573 | 10000 | 501187.2 | 5047.659 | 5047.659 | 5047.659 | 501187.2336 |
| | std. dev. | | 3.981072 | 63.09573 | 2.511886 | 3.184857 | 3.184857 | 3.184857 | 2.511886432 |
| | distrib. | constant | triangular | triangular | triangular | triangular | triangular | triangular | triangular |
| Selenium (+6) | min | | 0.501187 | 10 | 6309.573 | 0.40095 | 0.40095 | 0.40095 | 6309.573445 |
| | mean | 0 | 19.95262 | 3981.072 | 25118.86 | 15.9621 | 15.9621 | 15.9621 | 25118.86432 |
| | max | | 251.1886 | 10000 | 63095.73 | 200.9509 | 200.9509 | 200.9509 | 63095.73445 |
| | std. dev. | | 2.511886 | 15.84893 | 2.511886 | 2.009509 | 2.009509 | 2.009509 | 2.511886432 |
| | distrib. | constant | triangular | triangular | triangular | triangular | triangular | triangular | triangular |

(continued)

Table 17A-2b. (continued)

| Chemical | Statistic | Environmental Media Kd Values (L/kg) | | | | Waste Kd Values (L/kg) | | | | |
|----------|-----------|--------------------------------------|------------|------------|---------------|------------------------|------------|------------|---------------------|--------------|
| | | Organic carbon | Soil | Sediment | Surface Water | LAU | Waste Pile | Landfill | Surface Impoundment | Aerated Tank |
| Silver | min | | 10 | 125.8925 | 25118.86 | 8 | 8 | 8 | 25118.86432 | 25118.86 |
| | mean | 0 | 398.1072 | 3981.072 | 158489.3 | 318.4857 | 318.4857 | 318.4857 | 158489.3192 | 158489.3 |
| | max | | 31622.78 | 630957.3 | 1995262 | 25298.22 | 25298.22 | 25298.22 | 1995262.315 | 1995262 |
| | std. dev. | | 6.309573 | 12.58925 | 3.981072 | 5.047659 | 5.047659 | 5.047659 | 3.981071706 | 3.981072 |
| | distrib. | constant | triangular | triangular | triangular | triangular | triangular | triangular | triangular | triangular |
| Thallium | min | | 0.063096 | 0.316228 | 1000 | 0.050477 | 0.050477 | 0.050477 | 1000 | 1000 |
| | mean | 0 | 3.162278 | 19.95262 | 12589.25 | 2.529822 | 2.529822 | 2.529822 | 12589.25412 | 12589.25 |
| | max | | 31.62278 | 3162.278 | 31622.78 | 25.29822 | 25.29822 | 25.29822 | 31622.7766 | 31622.78 |
| | std. dev. | | 7.943282 | 12.58925 | 10 | 6.354626 | 6.354626 | 6.354626 | 10 | 10 |
| | distrib. | constant | triangular | triangular | triangular | triangular | triangular | triangular | triangular | triangular |
| Vanadium | min | | 3.162278 | 2.511886 | 316.2278 | 2.529822 | 2.529822 | 2.529822 | 316.227766 | 316.2278 |
| | mean | 0 | 50.11872 | 125.8925 | 5011.872 | 40.09498 | 40.09498 | 40.09498 | 5011.872336 | 5011.872 |
| | max | | 316.2278 | 1584.893 | 31622.78 | 252.9822 | 252.9822 | 252.9822 | 31622.7766 | 31622.78 |
| | std. dev. | | 31.62278 | 7.943282 | 3.981072 | 25.29822 | 25.29822 | 25.29822 | 3.981071706 | 3.981072 |
| | distrib. | constant | triangular | triangular | triangular | triangular | triangular | triangular | triangular | triangular |
| Zinc | min | 3.98E+04 | 0.1 | 31.62278 | 3162.278 | 0.08 | 0.08 | 0.08 | 3162.27766 | 3162.278 |
| | mean | 7.94E+04 | 501.1872 | 12589.25 | 100000 | 400.9498 | 400.9498 | 400.9498 | 100000 | 100000 |
| | max | 2.51E+06 | 100000 | 1584893 | 7943282 | 80000 | 80000 | 80000 | 7943282.347 | 7943282 |
| | std. dev. | | 10 | 39.81072 | 3.162278 | 8 | 8 | 8 | 3.16227766 | 3.162278 |
| | distrib. | constant | triangular | triangular | triangular | triangular | triangular | triangular | triangular | triangular |

**Table 17A-3. Aerobic Biodegradation Rates
(AerBio.csv)**

| Name | Aerobic biodegradation rate (1/day) | | | Distribution type | Reaction product |
|----------------------------|-------------------------------------|----------|----------|-------------------|------------------|
| | min | central | max. | | |
| Acetone | 0 | 0.035 | 1.2 | Uniform | |
| Benzene | 0 | 0.096 | 3.3 | Uniform | |
| Benzo(a)anthracene | 0.000096 | 0.0035 | 0.072 | Uniform | |
| Benzo(a)pyrene | 0 | 0.0027 | 0.057 | Uniform | |
| Bis(2-ethylhexyl)phthalate | 0 | 0.0205 | 0.23 | Uniform | |
| Chrysene | 0 | 0.003 | 0.037 | Uniform | |
| m-Cresol | 0.0035 | 0.133 | 1.16 | Uniform | |
| o-Cresol | 0.069 | 0.4 | 4.61 | Uniform | |
| p-Cresol | 0.079 | 1.75 | 13.15 | Uniform | |
| Dichloromethane | 0.00362 | 0.0546 | 0.533 | Uniform | |
| Ethylbenzene | 0.003 | 0.113 | 4.8 | Uniform | |
| Fluoranthene | 0 | 0.0048 | 0.045 | Uniform | |
| Fluorene | 0.0018 | 0.015 | 0.33 | Uniform | |
| Methanol | 0 | 0.118 | 0.693 | Uniform | |
| Methyl ethyl ketone | 0.4 | 0.69 | 1.4 | Uniform | |
| Naphthalene | 0 | 0.308 | 5 | Uniform | |
| Phenol | 0.024 | 0.21 | 11 | Uniform | |
| Pyrene | 0 | 0.00345 | 0.052 | Uniform | |
| Tetrachloroethylene | 0 | 0 | 0.139 | Uniform | |
| Toluene | 0 | 0.2 | 42.5 | Uniform | |
| m-Xylene | 0 | 0.057 | 0.76 | Uniform | |
| o-Xylene | 0 | 0.054 | 7.625 | Uniform | |
| p-Xylene | 0 | 0.052 | 0.56 | Uniform | |
| Divalent Mercury | 1.00E-05 | 5.00E-04 | 5.00E-03 | Triangular | Methyl Mercury |
| Methyl Mercury | 1.00E-04 | 5.00E-03 | 5.00E-02 | Triangular | Divalent Mercury |

Table 17A-4. Anaerobic Biodegradation Rates (AnaBio.csv)

| Chemical | Anaerobic Biodegradation Rate (k_bio, 1/day) ¹ | | | | Distribution Type | Reaction Product |
|---|--|---------|---------|-----------|-------------------|------------------|
| | minimum | mean | maximum | std. dev. | | |
| Acenaphthalene | 0.0043 | 0.0043 | 0.0043 | | Constant | |
| Benzene | 0 | 0 | 0.071 | 0.0152 | Uniform | |
| 1,1'-Biphenyl | 0 | 0.00016 | 0.019 | 0.00944 | Uniform | |
| Carbon tetrachloride | 0 | 0.16343 | 1.73 | 0.572 | Uniform | |
| Chloroform | 0.004 | 0.0315 | 0.25 | 0.0884 | Uniform | |
| m-Cresol | 0.0029 | 0.029 | 0.033 | 0.0138 | Uniform | |
| o-Cresol | 0 | 0.005 | 0.034 | 0.0172 | Uniform | |
| p-Cresol | 0.035 | 0.037 | 0.048 | 0.007 | Uniform | |
| Cumene | 0 | 0 | 0 | | Constant | |
| Dichlorodifluoromethane (CFC-12) | 0 | 0 | 0 | | Constant | |
| 1,2-Dichloroethane | 0.0076 | 0.0076 | 0.0076 | | Constant | |
| Dichloromethane | 0.0064 | 0.0064 | 0.0064 | | Constant | |
| 2,4-Dichlorophenol | 0 | 0.016 | 0.12 | 0.0501 | Uniform | |
| Dioxane | 0 | 0 | 0 | | Constant | |
| Ethylbenzene | 0 | 0.0031 | 0.46 | 0.0762 | Uniform | |
| Fluorene | 0 | 0.00015 | 0.00145 | 0.00069 | Uniform | |
| Methanol | 0 | 0.036 | 0.34 | 0.0697 | Uniform | |
| 1-Methylnaphthalene | 0 | 0 | 0.057 | 0.0214 | Uniform | |
| Naphthalene | 0 | 0 | 0.03 | 0.00791 | Uniform | |
| Nitrobenzene | 0.0037 | 0.0037 | 0.1168 | 0.0427 | Uniform | |
| Pentachlorophenol | 0 | 0 | 0 | 0 | Constant | |
| Phenol | 0 | 0.032 | 0.2 | 0.0651 | Uniform | |
| Pyridine | 0 | 0.01 | 0.02 | 0.0102 | Uniform | |
| Styrene | 0 | 0 | 0 | | Constant | |
| Tetrachloroethylene | 0 | 0.00186 | 0.071 | 0.0223 | Uniform | |
| Toluene | 0 | 0.02 | 0.186 | 0.0372 | Uniform | |
| 1,1,2-Trichloro-1,2,2-trifluoroethane (CFC-113) | 0 | 0 | 0 | | Constant | |
| 1,1,1-Trichloroethane | 0 | 0.00355 | 0.041 | 0.013 | Uniform | |

(continued)

Table 17A-4. (continued)

| Chemical | Anaerobic Biodegradation Rate (k_bio, 1/day) ¹ | | | | Distribution Type | Reaction Product |
|------------------------------------|--|----------|----------|-----------|-------------------|------------------|
| | minimum | mean | maximum | std. dev. | | |
| Trichloroethylene | 0.00082 | 0.0016 | 0.04 | 0.00889 | Uniform | |
| Trichlorofluoromethane (CFC-11) | 0.0016 | 0.0016 | 0.0016 | | Constant | |
| 1,3,5-Trimethylbenzene | 0 | 0 | 0.0039 | 0.00174 | Uniform | |
| Vinyl Chloride | 0 | 0.00405 | 0.0582 | 0.0139 | Uniform | |
| m-Xylene | 0 | 0.006 | 0.32 | 0.0675 | Uniform | |
| o-Xylene | 0 | 0.004 | 0.21 | 0.0468 | Uniform | |
| p-Xylene | 0 | 0.0052 | 0.17 | 0.0367 | Uniform | |
| Divalent mercury | 1.00E-05 | 1.00E-04 | 1.00E-03 | | Triangular | Methyl mercury |
| Methyl mercury | 5.00E-05 | 5.00E-04 | 5.00E-03 | | Triangular | Divalent mercury |

¹ Same rates for all pH and temperature regimes

Table 17A-5. Anaerobic Biodegradation Rates, Reducing Conditions (AnaRed.csv)

| Chemical | Anaerobic biodegradation rate (k_bio, 1/d) | | | | Degradation Product |
|-------------------|--|----------|----------|-------------------|---------------------|
| | minimum | mean | maximum | distribution type | |
| Divalent mercury | 5.00E-03 | 1.00E-02 | 1.00E-01 | triangular | Elemental mercury |
| Methyl mercury | 1.00E-05 | 1.00E-03 | 1.00E-02 | triangular | Elemental mercury |
| Elemental mercury | 1.00E-05 | 1.00E-03 | 1.00E-02 | triangular | Divalent mercury |

**Table 17A-6a. Anaerobic Biodegradation Rates:
Methanogenic Conditions (MethBio.csv)
[statistical distributions, all pH and temperature regimes]**

| Chemical | Distribution type | Anaerobic biodegradation rate (k_bio, 1/d) | | | |
|---|-------------------|--|---------|---------|-----------|
| | | minimum | mean | maximum | std. dev. |
| Acenaphthalene | Constant | 0.0043 | 0.0043 | 0.0043 | |
| 1,1'-Biphenyl | Uniform | 0 | 0.00016 | 0.019 | 0.00944 |
| Carbon tetrachloride | Uniform | 0 | 0.16343 | 1.73 | 0.572 |
| m-Cresol | Uniform | 0.0029 | 0.029 | 0.033 | 0.0138 |
| o-Cresol | Uniform | 0 | 0.005 | 0.034 | 0.0172 |
| p-Cresol | Uniform | 0.035 | 0.037 | 0.048 | 0.007 |
| Cumene | Constant | 0 | 0 | 0 | |
| Dichlorodifluoromethane (CFC-12) | Constant | 0 | 0 | 0 | |
| 1,2-Dichloroethane | Constant | 0.0076 | 0.0076 | 0.0076 | |
| 2,4-Dichlorophenol | Uniform | 0 | 0.016 | 0.12 | 0.0501 |
| Dioxane | Constant | 0 | 0 | 0 | |
| Ethylbenzene | Uniform | 0 | 0.0031 | 0.46 | 0.0762 |
| Fluorene | Uniform | 0 | 0.00015 | 0.00145 | 0.00069 |
| Methanol | Uniform | 0 | 0.036 | 0.34 | 0.0697 |
| 1-Methylnaphthalene | Uniform | 0 | 0 | 0.057 | 0.0214 |
| Naphthalene | Uniform | 0 | 0 | 0.03 | 0.00791 |
| Styrene | Constant | 0 | 0 | 0 | |
| 1,1,2-Trichloro-1,2,2-trifluoroethane (CFC-113) | Constant | 0 | 0 | 0 | |
| Trichlorofluoromethane (CFC-11) | Constant | 0.0016 | 0.0016 | 0.0016 | |
| 1,3,5-Trimethylbenzene | Uniform | 0 | 0 | 0.0039 | 0.00174 |
| m-Xylene | Uniform | 0 | 0.006 | 0.32 | 0.0675 |
| o-Xylene | Uniform | 0 | 0.004 | 0.21 | 0.0468 |
| p-Xylene | Uniform | 0 | 0.0052 | 0.17 | 0.0367 |

Table 17A-6b. Anaerobic Biodegradation Rates: Methanogenic Conditions (MethBio.csv)
[empirical distributions, by pH and temperature regime]

| Chemical | Anaerobic biodegradation rate (k_bio, 1/d) | | | | | | | | | | | | | |
|--------------------------------|--|----------|----------|-----------|--------|--------|----------|--------|-------|---------|-------|----------|-------|-------|
| | min. | mean | max. | std. dev. | p5 | p6 | p7 | p8 | p9 | p10 | p11 | p12 | p13 | p14 |
| <i>T<15, pH<6</i> | | | | | | | | | | | | | | |
| Benzene | 0 | 0 | | | | | | | | | | | | |
| Toluene | 0.043 | 0 | | | | | | | | | | | | |
| Tetrachloroethylene | | 0 | | | | | | | | | | | | |
| 1,1,1-Trichloroethane | | 0.011 | | | | | | | | | | | | |
| Trichloroethylene | | 0 | | | | | | | | | | | | |
| Nitrobenzene | | 0.0037 | | | | | | | | | | | | |
| Pentachlorophenol | 1.41E-03 | 1.98E-03 | | | | | | | | | | | | |
| <i>T<15, 6<=pH<=8</i> | | | | | | | | | | | | | | |
| Benzene | 0 | 0 | 0 | 0 | 0 | 0 | 0.000108 | 0.0015 | 0.002 | 0.00714 | 0.017 | 0.031 | 0.052 | 0.071 |
| Toluene | 0 | 0 | 0 | 0.042 | 0.042 | 0.043 | 0.0532 | 0.093 | 0.1 | 0.186 | | | | |
| Tetrachloroethylene | 0 | 0 | 0.000735 | 0.0109 | 0.071 | | | | | | | | | |
| 1,1,1-Trichloroethane | 0 | 0.0013 | 0.0037 | 0.0375 | 0.041 | | | | | | | | | |
| Trichloroethylene | 0 | 0 | 0 | 0.00062 | 0.0023 | 0.0034 | | | | | | | | |
| Nitrobenzene | | | | | | | | | | | | | | |
| Pentachlorophenol | | 1.97E-03 | | | | | 4.94E-03 | | | | 0 | 5.09E-03 | 0 | |
| Phenol | | 0 | | | | | 0.13 | | | | 0.57 | 0.1 | | |
| Pyridine | | | | | | | | | | | 0.01 | | | |
| Dichloromethane | | 0.0064 | | | | | | | | | | | | |
| Vinyl Chloride | 0.00093 | 0.00297 | | | | | | | | | | | | |

(continued)

Table 17A-6b. (continued)

| Chemical | Anaerobic biodegradation rate (k_bio, 1/d) | | | | | | | | | | | | |
|---------------------------------|--|----------|-------|-----------|--------|--------|-------|--------|-------|-------|-----|-----|-----|
| | min. | mean | max. | std. dev. | p5 | p6 | p7 | p8 | p9 | p10 | p11 | p12 | p13 |
| T<15, pH>8 | | | | | | | | | | | | | |
| Pentachlorophenol | | 5.75E-03 | | | | | | | | | | | |
| Vinyl chloride | 0 | | | | | | | | | | | | |
| T>=15, pH<6 | | | | | | | | | | | | | |
| Trichloroethylene | | 0 | | | | | | | | | | | |
| T>=15, 6<=pH<=8 | | | | | | | | | | | | | |
| Benzene | 0 | 0 | 0 | 0 | 0 | 0 | 0.005 | 0.0074 | | | | | |
| Toluene | 0 | 0 | 0 | 0.003 | 0.0098 | 0.0115 | 0.018 | 0.028 | 0.032 | 0.034 | | | |
| Tetrachloroethylene | 0.0084 | 0.003 | | | | | | | | | | | |
| 1,1,1-Trichloroethane | | 0.0092 | | | | | | | | | | | |
| Trichloroethylene | 0.039 | 0.016 | 0.013 | | | | | | | | | | |

Table 17A-7. Anaerobic Biodegradation Rates - Sulfate Reducing Conditions (SO4Bio.csv)

| Chemical | Distribution type | Anaerobic biodegradation rates (k_bio, 1/d) | | | | p5 | p6 | p7 | p8 |
|---|-------------------|---|---------|---------|-----------|----|----|----|----|
| | | minimum | mean | maximum | std. dev. | | | | |
| <i>All pH and Temperature conditions</i> | | | | | | | | | |
| Acenaphthalene | Constant | 0.0043 | 0.0043 | 0.0043 | | | | | |
| 1,1'-Biphenyl | Uniform | 0 | 0.00016 | 0.019 | 0.00944 | | | | |
| Carbon Tetrachloride | Uniform | 0 | 0.16343 | 1.73 | 0.572 | | | | |
| m-Cresol | Uniform | 0.0029 | 0.029 | 0.033 | 0.0138 | | | | |
| o-Cresol | Uniform | 0 | 0.005 | 0.034 | 0.0172 | | | | |
| p-Cresol | Uniform | 0.035 | 0.037 | 0.048 | 0.007 | | | | |
| Cumene | Constant | 0 | 0 | 0 | | | | | |
| Dichlorodifluoromethane (CFC-12) | Constant | 0 | 0 | 0 | | | | | |
| 1,2-Dichloroethane | Constant | 0.0076 | 0.0076 | 0.0076 | | | | | |
| 2,4-Dichlorophenol | Uniform | 0 | 0.016 | 0.12 | 0.0501 | | | | |
| Dioxane | Constant | 0 | 0 | 0 | | | | | |
| Ethylbenzene | Uniform | 0 | 0.0031 | 0.46 | 0.0762 | | | | |
| Fluorene | Uniform | 0 | 0.00015 | 0.00145 | 0.00069 | | | | |
| Methanol | Uniform | 0 | 0.036 | 0.34 | 0.0697 | | | | |
| 1-Methylnaphthalene | Uniform | 0 | 0 | 0.057 | 0.0214 | | | | |
| Naphthalene | Uniform | 0 | 0 | 0.03 | 0.00791 | | | | |
| Styrene | Constant | 0 | 0 | 0 | | | | | |
| 1,1,2-Trichloro-1,2,2-trifluoroethane (CFC-113) | Constant | 0 | 0 | 0 | | | | | |

(continued)

Table 17A-7. (continued)

| Chemical | Distribution type | Anaerobic biodegradation rates (k_bio, 1/d) | | | | p5 | p6 | p7 | p8 |
|---------------------------------|-------------------|---|---------|---------|-----------|--------|--------|--------|-------|
| | | minimum | mean | maximum | std. dev. | | | | |
| Trichlorofluoromethane (CFC-11) | Constant | 0.0016 | 0.0016 | 0.0016 | | | | | |
| 1,3,5-Trimethylbenzene | Uniform | 0 | 0 | 0.0039 | 0.00174 | | | | |
| m-Xylene | Uniform | 0 | 0.006 | 0.32 | 0.0675 | | | | |
| o-Xylene | Uniform | 0 | 0.004 | 0.21 | 0.0468 | | | | |
| p-Xylene | Uniform | 0 | 0.0052 | 0.17 | 0.0367 | | | | |
| T<15, pH<6 | | | | | | | | | |
| Benzene | Demp | | 0 | | | | | | |
| Phenol | Demp | | 0.2 | | | | | | |
| Toluene | Demp | | 0 | | | | | | |
| T<15 6<=pH<=8 | | | | | | | | | |
| Benzene | Demp | 0 | 0 | 0.00134 | 0.0029 | 0.0041 | 0.0063 | 0.0065 | 0.047 |
| NitroBenzene | Demp | | 0.00263 | | | | | | |
| Phenol | Demp | 0 | 0.0135 | | | | | | |
| Tetrachloroethylene | Demp | 0 | 0.00405 | | | | | | |
| Toluene | Demp | 0.0045 | 0.0024 | 0.01 | 0.016 | 0.019 | 0.066 | 0.083 | 0.087 |
| 1,1,1-Trichloroethane | Demp | 0 | 0 | 0.01 | | | | | |
| Trichloroethylene | Demp | 0.00086 | 0.00074 | 0.0013 | 0.00231 | 0.0033 | 0.0036 | 0.01 | 0.014 |
| Vinyl Chloride | Demp | | 0.0008 | | | | | | |

(continued)

Table 17A-7. (continued)

| Chemical | Distribution type | Anaerobic biodegradation rates (k_bio, 1/d) | | | | p5 | p6 | p7 | p8 |
|---------------------------------|-------------------|---|---------|---------|-----------|--------|-------|------|----|
| | | minimum | mean | maximum | std. dev. | | | | |
| <i>T>=15, pH<6</i> | | | | | | | | | |
| Benzene | Demp | | 0 | | | | | | |
| Chloroform | Demp | | 0.01562 | | | | | | |
| Pentachlorophenol | Demp | | 0 | | | | | | |
| Tetrachloroethylene | Demp | | 0.00073 | | | | | | |
| Toluene | Demp | | 0.0086 | | | | | | |
| Trichloroethylene | Demp | 0 | 0.0011 | | | | | | |
| <i>T>=15, 6<=pH<=8</i> | | | | | | | | | |
| Benzene | Demp | 0 | 0.003 | 0.0041 | 0.0237 | 0.0308 | | | |
| Chloroform | Demp | 0.03 | 0.142 | | | | | | |
| Pyridine | Demp | | 0.014 | | | | | | |
| Tetrachloroethylene | Demp | 0.0065 | 0.054 | | | | | | |
| Toluene | Demp | 0.011 | 0.018 | 0.027 | 0.0446 | 0.045 | 0.091 | 0.11 | |
| 1,1,1-Trichloroethane | Demp | 0.003 | 0.0092 | 0.0099 | | | | | |
| Trichloroethylene | Demp | 0.00069 | 0.0015 | 0.00153 | 0.0029 | 0.003 | 0.009 | 0.01 | |
| Vinyl Chloride | Demp | 0.0069 | 0.0082 | | | | | | |

Demp = empirical distribution

Table 17A-8. Catalyzed Hydrolysis Rates (CAT.csv)

| Chemical | Hydrolysis rate | Reaction Products | | |
|---|-----------------|---|---------------------------------|-------------------|
| | | 1 | 2 | 3 |
| <i>Acid Hydrolysis Rates (k_HA, L/mole-day)</i> | | | | |
| Acrylonitrile | 1.368925394 | Acrylamide | | |
| <i>Neutral Hydrolysis Rates (k_HN, 1/day)</i> | | | | |
| Chloroform | 0.000000274 | Carbon monoxide | Hydrochloric acid | |
| Ethylene dibromide | 0.001724846 | Hydrobromic acid | Vinyl bromide | 2-Bromoethanol |
| Methoxychlor | 0.001889117 | 2,2-Bis(p-methoxyphenyl)-1,1-dichloroethylene | Anisoin | Hydrochloric acid |
| Methylene chloride | 0.00000274 | Formaldehyde | Hydrochloric acid | |
| Thiram | 0.119917864 | -- | | |
| 1,1,1-Trichloroethane | 0.001752225 | 1,1-Dichloroethylene | Acetic acid | Hydrochloric acid |
| <i>Base Hydrolysis Rates (k_HB, L/mole-day)</i> | | | | |
| Acetonitrile | 0.123203285 | Acetamide | | |
| Acrylonitrile | 14.23682409 | Acrylamide | | |
| Bis-(2-ethylhexyl) phthalate | 3.832991102 | 2-Ethylhexanol | 2-Ethylhexyl hydrogen phthalate | |
| Carbon disulfide | 86.24229979 | Carbonyl sulfide | | |
| Chloroform | 7.501711157 | Carbon monoxide | Hydrochloric acid | |
| Methoxychlor | 32.85420945 | 2,2-Bis(p-methoxyphenyl)-1,1-dichloroethylene | Anisoin | Hydrochloric acid |
| Methyl methacrylate | 5201.916496 | Methacrylic acid | Methanol | |
| Methylene chloride | 0.00164271 | Formaldehyde | Hydrochloric acid | |
| Thiram | 99657.76865 | -- | | |
| 1,1,1-Trichloroethane | 6570.841889 | 1,1-Dichloroethylene | Acetic acid | Hydrochloric acid |